WE CLAIM:

1. A system for electronically managing, finding, and/or visualizing biomolecular interactions comprising a computer system including at least one computer receiving data on biomolecular interactions from a plurality of providers and processing such data to create and maintain images and/or text defining biomolecular interactions, said computer system, in response to data requests, creating and transmitting to a plurality of end-users, the images and/or text defining biomolecular interactions.

2. A system as claimed in claim 1 wherein the biomolecular interaction comprises a protein, nucleic acid, ligand, molecular complex, and signaling pathway.

3. A system as claimed in claim 1 wherein the biomolecular interactions are defined by chemical graphs.

4. . A method for displaying on a computer screen information concerning biomolecular interactions comprising retrieving an image and/or text defining a biomolecular interaction from a system as claimed in claim 1.

5. A data structure stored in the memory of a computer the data structure having a plurality of records and each record containing a biomolecular interaction defined by a chemical graph and information relating to the biomolecular interaction.

6. A data structure as claimed in claim 5 wherein the information is accessible by using indices representing selections of information from the chemical graph.

7. A method for storing a representation of a biomolecular interaction in a memory of a computer system, the method executed on a computer system and comprising the steps of:
   (a) identifying a chemical graph of a biomolecular interaction; and
   (b) storing a record in a data structure as claimed in claim 5.

8. A method for storing a representation of a biomolecular interaction in a memory of a computer system, the method executed on a computer system and comprising the steps of:
   (a) identifying a chemical graph of a biomolecular interaction;
   (b) generating one or more indices from information in the chemical graph; and
   (c) storing a record in a data structure as claimed in claim 6.

9. A method for identifying a biomolecular interaction that is similar to a reference biomolecular interaction, the method executed on a computer and comprising the steps of:

(a) conducting a similarity search for each molecule in a test biomolecular interaction;

(b) screening the results of the similarity search;

(c) assembling a putative biomolecular interaction to create a test record;

(d) accessing one or more records in a data structure stored in the memory, the data structure having a plurality of records, each of the records containing a reference biomolecular interaction and information relating to the reference biomolecular interaction; and

(e) matching the test record with each record in the data structure to produce a matching record containing a reference biomolecular interaction matching the test biomolecular interaction.

10. A computer system for storing a representation of one or more biomolecular interactions in a memory in the computer system and for comparing one or more reference biomolecular interactions to a test biomolecular interaction, comprising:

(a) a database means stored in the memory representing one or more biomolecular interactions, each of the biomolecular interactions represented by a chemical graph; and

(b) a data structure means for storing a plurality of record means, each record means containing a chemical graph of the test biomolecular interaction.

11. A computer system comprising memory means, storage means, program means, and stored means for representing virtual-models of biomolecular interactions in the computer system comprising:

(a) one or more libraries of reference biomolecular interactions that comprise any number of attributes or components of the biomolecular interactions which values are either being used to describe characteristics of the types of biomolecular interactions in the computer system, or values or data structures used by the program at runtime, or are to be used to more specifically describe characteristics of individual components of the biomolecular interaction that each instance of a type of biomolecular interaction is to represent, or characteristics of each instance of a biomolecular interaction in the computer system; wherein the attributes have values of any type in the computer system or in a network accessible by the computer system;

(b) means for manipulating the biomolecular interaction by domain experts or program means comprising visual means for making the biomolecular interactions available through menus or palettes or programmatic means; and

(c) constructor means to create new instances from the definitions of the biomolecular interactions, and means to establish directional output-input links between complemenatary instances of the biomolecular interactions directly or through components.

12. A computer system comprising:

(a) a database having a plurality of records, each of said records containing a reference biomolecular interaction defined by a chemical graph and descriptive information from an external database which information correlates the biomolecular interactions to records in the external database; and

(b) a user interface allowing a user to selectively view information regarding a biomolecular interaction.

13. A computer system as claimed in claim 12 comprising:

(a) a database having a plurality of records, each of said records containing a reference biomolecular interaction defined by a chemical graph and descriptive information from an external database, which information correlates the biomolecular interactions to records in the external database;

(b) a processor in communication with said database and responsive to user input to access records in said database; and

(c) a user interface allowing a user to provide user input to said processor to selectively view information regarding a biomolecular interaction.

14. A computer system as claimed in claim 13 wherein the external database is PubMed.

15. A computer system as claimed in claim 13 wherein the records are encoded by standard data grammars.

16. A computer system as claimed in claim 13 wherein the records are encoded in ASN.1 or XML.

17. A computer system as claimed in claim 13 wherein the user interface further comprises user selectable links to enable a user to access additional information for a biomolecular interaction.

18. A computer system as claimed in claim 17 wherein the links comprise HTML links.

19. A method for presenting information pertaining to records of biomolecular interactions in a computer database, the records containing information identifying the biomolecular interactions and defining the biomolecular interactions by chemical graphs, the method comprising the steps of:

(a) providing an interface for entering query information relating to a biomolecular interaction;

(b) examining records in said database to locate data corresponding to the entered query information; and

(c) displaying the data corresponding to the entered query information.

20. A computer program product comprising a computer-usable medium having computer-readable program code embodied thereon relating to a plurality of records of biomolecular interactions, the records identifying the biomolecular interactions and defining chemical graphs of the biomolecular interactions, the computer program product comprising computer-readable program code for effecting the following steps within a computing system:
    (a) providing an interface for entering query information relating to a biomolecular interaction;
    (b) locating data corresponding to the entered query information; and
    (c) displaying the data corresponding to the entered query information.

21. A database system comprising a plurality of internal records, the database comprising a plurality of records, wherein each record contains a reference biomolecular interaction defined by chemical graphs and descriptive information from an external database which information correlates the biomolecular interactions to records in the external database.

22. . A database storing data relating to biomolecular interactions comprising:
    (a) first data types describing biomolecular interactions between chemical objects;
    (b) second data types describing collections of biomolecular interactions; and
    (c) third data types describing pathways between said collections of interactions.

23. A database as claimed in claim 22 wherein each of said first data types includes objects for said chemical objects, each of said objects including at least one of a pointer to an external database describing the chemical object, a sequence, and a chemical graph.

24. A database as claimed in claim 23 wherein the first data types are stored as records and further including objects identifying the biomolecular interactions and defining chemical graphs of the biomolecular interactions.

25. A database as claimed in claim 24 wherein the second data types include lists of identifications referencing the biomolecular interactions in said collections.

26. A database as claimed in claim 25 wherein said third data types include objects for said chemical objects that can form networks of interactions.

27. A database as claimed in claim 26 wherein said networks of interactions include metabolic pathways and cell signaling pathways.

28. A database as claimed in claim 27 wherein third data types include sequences of identifications referencing biomolecular interactions that make up said pathways.